Anomalous Structural Phase Transitions in $SrTiO_3$ Thin Films

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X22A, X22C

Introduction: Strains induced in thin films often cause their properties to be much different from the bulk material of the same composition. For many materials, relatively little is known of the details of the underlying structural changes that lead to such altered properties. Our work is focused on measuring the structure of perovskite titanates under a variety of different strain conditions. Particular attention has been paid to the cubic to tetragonal (c-t) phase transition in $SrTiO_3$ that occurs in bulk material near 105 K. The titanates have important physical properties such as ferroelectricity and variable dielectric constants. They can also be considered as parent compounds for a variety of complex oxides currently under intense study such as high temperature superconductors and colossal magnetoresistance materials.

Methods and Materials: The samples were grown at Penn State University using pulsed laser deposition onto heated substrates. We have studied $SrTiO_3$ films in three types of structures; $SrTiO_3$ on a $LaAlO_3$ with a $SrRuO_3$ buffer layer (STO/SRO/LAO), $SrTiO_3$ on $LaAlO_3$ with no buffer layer (STO/LAO), and $SrTiO_3$ on a $SrTiO_3$ substrate with a $SrRuO_3$ buffer layer (STO/SRO/STO). X-ray diffraction measurements were conducted at Beamlines X22A and X22C. Particular attention was paid toward measurement of the lattice constants and the intensity of the tetragonal superlattice peak.

Results: The Sto/SRO/LAO structure has the precise conditions for a highly strained film and thus exhibits a large change in the c-t transition temperature, from 105 K in the bulk to near 1000 K in the films, as shown in figure 1. The other two structures are less strained and show a c-t transition closer to the bulk value. This can be understood in the case of STO/LAO since the lattice mismatch is much larger, and thus we expect a great deal of interface defects leading to relieved strain in the film. The result appears to be a rounded transition near the bulk value caused by a range of strains, as shown in figure 2. The STO/SRO/STO system is more difficult to understand. We would expect it to be very similar to the STO/SRO/LAO. Measurements show it is in fact quite similar to the bulk, with a slight rise in the c-t transition temperature. Clearly the ultimate substrate exerts a significant long-range strain effect.

Conclusions: Our preliminary results show that lattice mismatch induced strains have a large effect on the structural phase transitions of oxide films. There is only a small amount of existing theory and at least one prediction that appears to qualitatively match our result [1], though many details and quantitative numbers appear to differ from prediction.

References: 1. N.A. Pertsev, A.K. Tagantsev, and N. Setter, Phys. Rev. B, 61, R825, (2000)

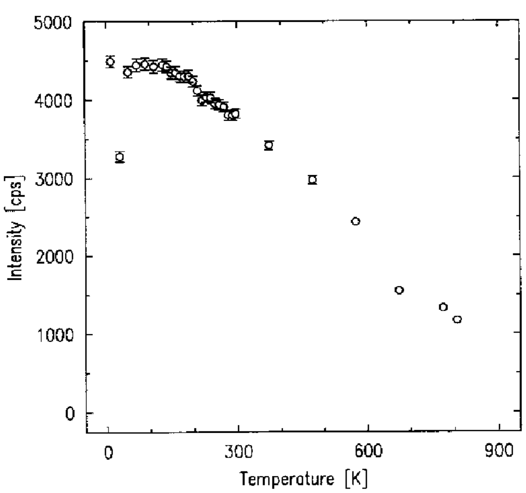

Figure 1. The STO tetragonal superlattice intensity for a STO/SRO/LAO structure. The intensity extrapolates to zero near 1000 K.

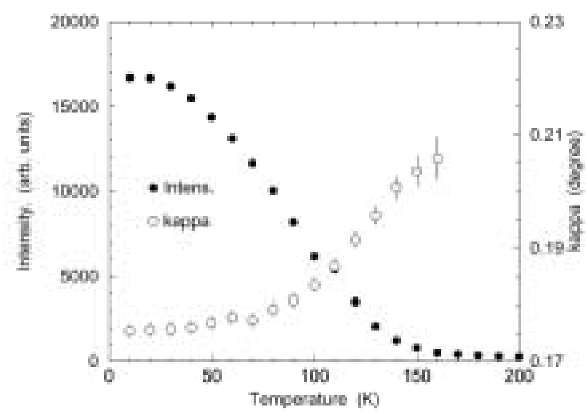

Figure 2. The STO tetragonal superlattice intensity for a STO/LAO structure. The transition is rounded and ranges from about 100 to 140 K.